

NEIGHBORHOOD-HISTORY QUANTUM WALK

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ABSTRACT. History dependent discrete time quantum walks (QWs) are often studied for their lattice traversal properties. A particular model, which we call the *site-history quantum walk* (SHQW), uses the state of a memory qubit at each site to record visits and to control the dynamics of the walk. We generalize this model to the *neighborhood-history quantum walk* (NHQW), in which the walk dynamics and the state of the memory qubits in a *neighborhood* of the particle's position are interdependent. To demonstrate it, we construct an NHQW on a one-dimensional lattice, with a simple neighborhood. Several dynamically interesting history dependent QWs, including the SHQW, can be realized as single-particle sectors of quantum lattice gas automata (QLGA). In contrast, the NHQW constructed in this paper is realized as a single-particle sector of the more general quantum cellular automaton (QCA). The complexity of the NHQW dynamics presents a promising avenue toward richer walk strategies.

1. INTRODUCTION

Discrete time quantum walks (QWs) have an established status as models of quantum search algorithms [1–5]. Being capable of universal quantum computation [6], they are contenders for quantum computing tasks as well. It is noteworthy that physical realizations of QWs have emerged, and as they develop further [7,8], they are useful for demonstrating and manipulating quantum behavior. Altogether, strong interest continues to grow in understanding and designing their lattice traversal properties [9–16] to achieve faster and more accurate search algorithms.

From a search standpoint, to perform a more efficient search with a QW, a desirable feature may be *self-avoidance*: reduced probability of visiting previously visited sites in favor of unvisited sites [12,13]. With this goal, a model of QW proposed by Camilleri *et al.* [12] expands the QW model to append a memory qubit to each lattice site, to maintain a record of particle visits. When the particle hops to a site, the interaction between the site's memory qubit and the particle modifies the memory qubit state and controls the particle direction for the next hop. We call this a *site-history quantum walk* (SHQW). We would like, instead, to make the particle interact with the neighboring memory qubits prior to the hop. That requires a further expansion of the QW model to bring the neighboring memories in interaction with the particle.

This paper is organized as follows. In Section 2 we give a brief description of the basic quantum walk (QW). In Section 3 we recall the site-history quantum walk (SHQW) from [12]. In Section 4 we introduce the *neighborhood-history quantum walk* (NHQW). In Section 5 we consider NHQWs over a simple neighborhood (left/right symmetric). First, we briefly describe a counterpart of SHQW for this neighborhood, and give a plausibility argument for why it would behave similarly to the SHQW. Then we move on to the NHQW

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scheme we are interested in, fundamentally different from SHQW, embodying internal (spin) parameters and external interaction parameters. This construction is related to the work in [19] on unentangled orthogonal bases (UOB). We show simulation results of the walk patterns obtained by choosing different sets of parameters. Adjusting these parameters leads to a range of walk behaviors. Next, we describe a quantum cellular automaton (QCA) whose restriction to a single-particle sector is this NHQW. It turns out that this QCA is a concatenation of QLGA, and such QCA are investigated in [20]. That paper studies QCA that have no particle description at the scale at which the dynamics are homogeneous. Section 6 concludes with some observations and future directions.

2. QUANTUM WALK

A QW consists of a quantum particle hopping on a lattice from site to site and scattering on arrival at the sites. Let us understand a basic QW on a one-dimensional finite sized lattice¹ of length N . We denote the lattice $\mathcal{L} = \mathbb{Z}_N$. The particle has a position on the lattice, $x \in \mathcal{L} = \mathbb{Z}_N$, and a velocity, $v \in \{+1, -1\}$, giving the direction of its next hop. The state of the particle is a unit vector in a Hilbert space with its basis elements labeled jointly by position and velocity, i.e., the QW Hilbert space is a tensor product of Hilbert spaces associated with position and velocity. The position Hilbert space, $\mathcal{H}_{\mathcal{L}} = \mathbb{C}^N$, is N -dimensional and has basis $\{|x\rangle : x \in \mathcal{L} = \mathbb{Z}_N\}$.² The velocity Hilbert space is two-dimensional, $\mathcal{H}_V = \mathbb{C}^2$, with basis $\{|v\rangle : v = +1, -1\}$. The $|+1\rangle$ velocity vector will be referred to as the *right-moving* and $|-1\rangle$ velocity vector as the *left-moving* on the lattice. Thus, the QW Hilbert space is

$$\mathcal{H} = \mathcal{H}_{\mathcal{L}} \otimes \mathcal{H}_V = \mathbb{C}^N \otimes \mathbb{C}^2.$$

State of the QW is a vector $\psi \in \mathcal{H}$ of unit norm $\|\psi\| = 1$.

At each time step, the state transitions in two successive stages:

(i) *Scattering* (or *coin toss*)

$$S = I \otimes U_S : |x\rangle |v\rangle \mapsto |x\rangle U_S(|v\rangle),$$

where U_S is a unitary map on the velocity space \mathbb{C}^2 . It is also commonly called a “coin” operator.

(ii) *Advection* (or *shift*)

$$A : |x\rangle |v\rangle \mapsto |x + v\rangle |v\rangle.$$

Here, the addition is modulo N to allow “wrap-around” at the edges of the lattice. The overall QW transition rule is denoted T , a composition of scattering followed by advection,

$$T = AS = A(I \otimes U_S).$$

3. SITE-HISTORY QUANTUM WALK

In [12], we are introduced to the notion of using memory qubits, one per lattice site, to record the history of visits, with $|0\rangle$ denoting the “not visited” state and $|1\rangle$ denoting the

¹Generalization to infinite lattice and multiple dimensions can be done through the framework in [17, 18].

² $\mathbb{Z}_N = \mathbb{Z}/(N)$.

“have visited” state. We call this walk the site-history QW (SHQW). For the lattice $\mathcal{L} = \mathbb{Z}_N$, the SHQW Hilbert space is

$$\mathcal{H} = \mathcal{H}_{\mathcal{L}} \otimes \mathcal{H}_V \otimes \bigotimes_{k \in \mathbb{Z}_N} \mathcal{H}_{M_k} = \mathbb{C}^N \otimes \mathbb{C}^2 \otimes \bigotimes_{k \in \mathbb{Z}_N} \mathbb{C}^2, \quad (1)$$

with $\mathcal{H}_{\mathcal{L}} = \mathbb{C}^N$, $\mathcal{H}_V = \mathbb{C}^2$, $\mathcal{H}_{M_k} = \mathbb{C}^2$, specifying Hilbert spaces corresponding to position, velocity, and memory qubit at position $k \in \mathbb{Z}_N$, respectively. We write a computational basis element of the Hilbert space \mathcal{H} as

$$|x\rangle |v\rangle |m_0 \dots m_{N-1}\rangle, \quad (2)$$

where $m_k \in \{0, 1\}$ denotes the memory qubit corresponding to site k .

Like QW, the SHQW transition is scattering followed by advection. Scattering happens in two stages. One stage updates the memory qubit on particle arrival at the site. The other stage performs a memory-controlled operation on the velocity. These operations are implicitly controlled by $|x\rangle$ which determines the memory location involved in the scattering.³

(i) Memory,

$$M : |x\rangle |v\rangle |m_0 \dots m_{N-1}\rangle \mapsto |x\rangle |v\rangle |m_0 \dots m_{x-1}\rangle U_M(|m_x\rangle) |m_{x+1} \dots m_{N-1}\rangle,$$

where U_M is a symmetric matrix,⁴ parameterized by θ_m (the memory strength),

$$U_M = \begin{pmatrix} \cos \theta_m & i \sin \theta_m \\ i \sin \theta_m & \cos \theta_m \end{pmatrix}.$$

(ii) Ricochet,

$$R : |x\rangle |v\rangle |m_0 \dots m_x \dots m_{N-1}\rangle \mapsto |x\rangle R_{m_x}(|v\rangle) |m_0 \dots m_x \dots m_{N-1}\rangle,$$

The state of the memory, m_x , determines the scattering R_{m_x} . For $m_x = 0$ (unvisited state), it is

$$R_0 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & i \\ i & 1 \end{pmatrix},$$

and for $m_x = 1$ (visited), it is the symmetric scattering matrix, in turn parameterized by θ_b (the “back action”),

$$R_1 = \begin{pmatrix} \cos \theta_b & i \sin \theta_b \\ i \sin \theta_b & \cos \theta_b \end{pmatrix}.$$

Scattering is the composition of the above operations

$$S = RM.$$

Advection acts as for the normal QW,

$$A : |x\rangle |v\rangle |m_0 \dots m_{N-1}\rangle \mapsto |x+v\rangle |v\rangle |m_0 \dots m_{N-1}\rangle.$$

SHQW transition is

$$T = AS.$$

In [12], numerical simulations of the SHQW for several instructive pairs of values of the parameters θ_m and θ_b are performed and discussed.

³This description of SHQW is the one in [18] adapted from the original in [12].

⁴All the matrices are assumed to be with respect to the specified bases for the respective Hilbert spaces.

4. NEIGHBORHOOD-HISTORY QUANTUM WALK

We expand the SHQW to define the neighborhood-history quantum walk (NHQW). The model is described in somewhat general terms. Denote by $\mathcal{L} = \mathbb{Z}_{N_1} \times \dots \times \mathbb{Z}_{N_n}$ the lattice on which the particle walks, so that each position basis element $|x\rangle$ is labeled by $x \in \mathcal{L}$. A velocity basis element $|v\rangle$ is labeled from some finite subset of the lattice: $v \in \mathcal{V} \subset \mathcal{L}$.

The Hilbert space of an NHQW is

$$\mathcal{H} = \mathcal{H}_{\mathcal{L}} \otimes \mathcal{H}_{\mathcal{V}} \otimes \bigotimes_{k \in \mathcal{L}} \mathcal{H}_{M_k} = \mathbb{C}^{|\mathcal{L}|} \otimes \mathbb{C}^{|\mathcal{V}|} \otimes \bigotimes_{k \in \mathcal{L}} \mathbb{C}^2.$$

$\mathcal{H}_{\mathcal{L}} = \mathbb{C}^{|\mathcal{L}|}$, $\mathcal{H}_{\mathcal{V}} = \mathbb{C}^{|\mathcal{V}|}$, $\mathcal{H}_{M_k} = \mathbb{C}^2$, correspond to Hilbert spaces for position, velocity, and memory qubit at position $k \in \mathcal{L}$, respectively. A basis element of this Hilbert space is given as

$$|x\rangle |v\rangle \bigotimes_{k \in \mathcal{L}} |m_k\rangle,$$

with $x \in \mathcal{L}$, $v \in \mathcal{V}$, and $m_k \in \{0, 1\}$.

In this model, we allow a set of memory elements from the sites surrounding every site to participate in the scattering. This is given by the *neighborhood* denoted by a finite subset of the lattice, $\mathcal{M} \subset \mathcal{L}$. The neighborhood of site x is just the neighborhood shifted to x : $\mathcal{M}_x = x + \mathcal{M}$.

An NHQW transition has the familiar steps of scattering (implicitly controlled by $|x\rangle$ through the neighborhood selection) and advection:

(i) Scattering,

$$S : |x\rangle |v\rangle \bigotimes_{k \in \mathbb{Z}_N} |m_k\rangle \mapsto |x\rangle \bigotimes_{l \in \mathcal{L} \setminus \mathcal{M}_x} |m_l\rangle U_S \left(|v\rangle \bigotimes_{k \in \mathcal{M}_x} |m_k\rangle \right),$$

where U_S is the *neighborhood scattering operator* acting unitarily on velocity and neighborhood memory Hilbert space: $\mathcal{H}_{\mathcal{V}} \otimes \bigotimes_{k \in \mathcal{M}_x} \mathcal{H}_{M_k}$

(ii) Advection,

$$A : |x\rangle |v\rangle \bigotimes_{k \in \mathbb{Z}_N} |m_k\rangle \mapsto |x+v\rangle |v\rangle \bigotimes_{k \in \mathbb{Z}_N} |m_k\rangle.$$

The NHQW transition is given as

$$T = AS.$$

Note 4.1. In the previous section, the neighborhood for SHQW was trivial, i.e., $\mathcal{M} = \{0\}$.

As an illustration of NHQW, we take the specific lattice and Hilbert space of the SHQW model, and include a neighborhood. Then we construct scattering operators that use that neighborhood.

5. NHQW WITH LEFT/RIGHT SYMMETRIC NEIGHBORHOOD

We take the lattice and Hilbert space of the SHQW given in eq. (1), and add the neighborhood in which the memory at the current site is not involved in the scattering, but the left/right neighbors are. This is the left/right symmetric neighborhood $\mathcal{M} = \{-1, +1\}$. If the current particle position is x , the neighboring memory locations are $\mathcal{M}_x = \{x-1, x+1\}$.

We first consider a memory-ricochet scattering for this neighborhood and then a scattering scheme conceived in a very different manner.

5.1. **A memory-ricochet NHQW.** The basic structure of the memory-ricochet scattering for this neighborhood is the same as that of the SHQW. The operations involved in the scattering are,

(i) Memory,

$$M : |x\rangle |v\rangle |m_0 \dots m_{N-1}\rangle \mapsto |x\rangle |v\rangle |m_x\rangle |m_0\rangle \dots \\ |m_{x-1}\rangle U_v(|m_{x-1}\rangle |m_{x+1}\rangle) |m_{x+1} \dots m_{N-1}\rangle,$$

where U_v is a symmetric matrix parameterized by θ_v , the memory strength,

$$U_v = \begin{pmatrix} \cos \theta_v & i \sin \theta_v \\ i \sin \theta_v & \cos \theta_v \end{pmatrix}.$$

(ii) Ricochet,

Denoting $\mathbf{m}_x = m_{x-1}m_{x+1}$, ricochet is

$$R : |x\rangle |v\rangle |m_0 \dots m_x \dots m_{N-1}\rangle \mapsto |x\rangle U_{\mathbf{m}_x}(|v\rangle) |m_0 \dots m_x \dots m_{N-1}\rangle,$$

where $U_{\mathbf{m}}$, $\mathbf{m} \in \{00, 01, 10, 11\}$, are parametrized as

$$U_{\mathbf{m}} = \begin{pmatrix} \cos \theta_{\mathbf{m}} & i \sin \theta_{\mathbf{m}} \\ i \sin \theta_{\mathbf{m}} & \cos \theta_{\mathbf{m}} \end{pmatrix},$$

and the parameter $\theta_{\mathbf{m}}$ is the back-action parameter corresponding to \mathbf{m} .

In terms of R and M the scattering is

$$S = RM.$$

Advection, A , is given as before,

$$A : |x\rangle |v\rangle |m_0 \dots m_{N-1}\rangle \mapsto |x+v\rangle |v\rangle |m_0 \dots m_{N-1}\rangle.$$

The overall transition is

$$T = AS.$$

In this model, the parameter θ_v determines the effect of the velocity on the neighborhood memory qubits through the memory operation M . Also, there are 4 possible neighborhood memory states, hence the back-action on velocity through the ricochet R is determined by the 4 back-action parameters $\{\theta_{\mathbf{m}}\}$. These give the walk a higher degree of maneuverability than SHQW. The fact that the two stages act independently, however, implies that the particle (velocity) has no “awareness” of the neighborhood memory state as it operates on them through M . Similarly, the neighborhood memory state acts on the velocity through R without “awareness” of the state of the velocity. Though this memory-ricochet scattering has more parameters than SHQW, its general behavior is expected to remain similar to that of SHQW.

We now create an NHQW with a scattering built from a basis of unentangled orthogonal vectors of the Hilbert space in eq. (1), i.e., an *unentangled orthogonal basis* (UOB).⁵ We call it the *UOB-scattering* NHQW.

⁵The characterization and construction of families of unentangled orthogonal bases (UOB) for multi-qubit systems is in [19].

5.2. UOB-scattering NHQW. We study a fundamentally different scheme for neighborhood dependence, one in which the scattering acts simultaneously on velocity and neighborhood memory.

The neighborhood scattering operator, U_S , acts on $\mathcal{H}_V \otimes \mathcal{M}_{x-1} \otimes \mathcal{M}_{x+1}$. First, we informally assign meaning to the neighborhood memory states $\{|m_{x-1}m_{x+1}\rangle\}$. We say that $|00\rangle, |11\rangle$ are the states from which the particle scatters in a “balanced” manner, and $|01\rangle, |10\rangle$ are the states from which the scattering is “unbalanced”. Note that the information about the scattering behavior is encoded in the pair $|m_{x-1}m_{x+1}\rangle$, and not individual memory qubits. Information about velocity relative to the neighborhood state is in the basis state $|v\rangle |m_{x-1}m_{x+1}\rangle$ of $\mathcal{H}_V \otimes \mathcal{M}_{x-1} \otimes \mathcal{M}_{x+1}$.

To ascribe explicitly the change experienced by the internal (spin) velocity and neighborhood states from the scattering relative to the pre-scattering basis states, we construct a UOB that carries the part of the scattering information related to the internal (spin) states of velocity and memory. In the interest of notational economy, we first encode the effect of scattering on the internal (spin) states through a parametrized *spin-transformation* notation. A spin-transformation with parameter η is a map of a basis $\{|b\rangle, |b\rangle^\perp\}$ of \mathbb{C}^2 to the basis

$$\begin{aligned} |b\rangle_\eta &= \cos \eta |b\rangle + i \sin \eta |b\rangle^\perp, \\ |b\rangle_\eta^\perp &= i \sin \eta |b\rangle + \cos \eta |b\rangle^\perp. \end{aligned} \quad (3)$$

We put this definition to use in defining the transformation of the internal (spin) states of velocity and memory. For velocity, we designate parameters α_0, α_1 for the spin states resulting from balanced scattering, and parameters β_0, β_1 for the unbalanced scatterings. Similarly we define spin parameters γ_l, γ_r (for left and right) that determine the behavior of the neighborhood memory qubits for both types of scatterings. The UOB is defined using the spin parameters just described, and the spin-transformation in eq. (3),

$$\{|j\rangle_{\alpha_0} |0\rangle_{\gamma_l} |1\rangle_{\gamma_r}, |j\rangle_{\alpha_1} |1\rangle_{\gamma_l} |0\rangle_{\gamma_r}, |j\rangle_{\beta_0} |1\rangle_{\gamma_l} |1\rangle_{\gamma_r}, |j\rangle_{\beta_1} |0\rangle_{\gamma_l} |0\rangle_{\gamma_r} : j \in \{+1, -1\}\}.$$

We also introduce external scattering parameters θ_0, θ_1 , involved in interactions that transform pairs of UOB elements in a manner akin to the spin transformation. Having defined the parameters and the UOB, we construct the neighborhood scattering operator U_S ,

$$\begin{aligned} U_S : | +1 \rangle | 00 \rangle &\mapsto \cos \theta_0 | +1 \rangle_{\alpha_0} | 0 \rangle_{\gamma_l} | 1 \rangle_{\gamma_r} + i \sin \theta_0 | -1 \rangle_{\alpha_1} | 1 \rangle_{\gamma_l} | 0 \rangle_{\gamma_r}, \\ | -1 \rangle | 00 \rangle &\mapsto i \sin \theta_0 | +1 \rangle_{\alpha_0} | 0 \rangle_{\gamma_l} | 1 \rangle_{\gamma_r} + \cos \theta_0 | -1 \rangle_{\alpha_1} | 1 \rangle_{\gamma_l} | 0 \rangle_{\gamma_r}, \\ | +1 \rangle | 01 \rangle &\mapsto | -1 \rangle_{\beta_0} | 1 \rangle_{\gamma_l} | 1 \rangle_{\gamma_r}, \\ | -1 \rangle | 10 \rangle &\mapsto | +1 \rangle_{\beta_0} | 1 \rangle_{\gamma_l} | 1 \rangle_{\gamma_r}, \\ | +1 \rangle | 10 \rangle &\mapsto | +1 \rangle_{\beta_1} | 0 \rangle_{\gamma_l} | 0 \rangle_{\gamma_r}, \\ | -1 \rangle | 01 \rangle &\mapsto | -1 \rangle_{\beta_1} | 0 \rangle_{\gamma_l} | 0 \rangle_{\gamma_r}, \\ | +1 \rangle | 11 \rangle &\mapsto \cos \theta_1 | +1 \rangle_{\alpha_1} | 1 \rangle_{\gamma_l} | 0 \rangle_{\gamma_r} + i \sin \theta_1 | -1 \rangle_{\alpha_0} | 0 \rangle_{\gamma_l} | 1 \rangle_{\gamma_r}, \\ | -1 \rangle | 11 \rangle &\mapsto i \sin \theta_1 | +1 \rangle_{\alpha_1} | 1 \rangle_{\gamma_l} | 0 \rangle_{\gamma_r} + \cos \theta_1 | -1 \rangle_{\alpha_0} | 0 \rangle_{\gamma_l} | 1 \rangle_{\gamma_r}. \end{aligned} \quad (4)$$

Notice that the scattering updates the neighboring memory qubits together with the velocity. This is a different form of scattering compared with the memory-ricochet model. It takes balanced neighborhoods to unbalanced neighborhoods and vice-versa. The post-scattering

velocity is “informed” by the pre-scattering neighborhood state and velocity. Conceptually, this scattering has the goal of implementing a reasonable search strategy.

In Figures 1-8, we show simulations of the NHQW for the parameter values in Table 1. The lattice size is $N = 13$. The initial state for each walk is ($\lfloor N/2 \rfloor$ is the center of the lattice)

$$\begin{aligned}\psi_0 &= \frac{1}{\sqrt{2}} | \lfloor N/2 \rfloor \rangle (|+1\rangle + |-1\rangle) \bigotimes^N |0\rangle \\ &= \frac{1}{\sqrt{2}} |6\rangle (|+1\rangle + |-1\rangle) \bigotimes^N |0\rangle.\end{aligned}$$

Each walk simulation is run for $\lfloor N/2 \rfloor = 6$ time steps. We plot the probability distribution that the particle is at position $x \in \mathbb{Z}_N$ at each time step (the velocity and memory tensor factors are traced out).

| | α_0 | α_1 | β_0 | β_1 | γ_l | γ_r | θ_0 | θ_1 |
|--------|------------|------------|-----------|-----------|------------|------------|------------|------------|
| Fig. 1 | 0 | 0 | $\pi/4$ | $\pi/4$ | $\pi/2$ | $\pi/2$ | $\pi/4$ | $\pi/4$ |
| Fig. 2 | 0 | 0 | 0 | 0 | 0 | 0 | $\pi/4$ | $\pi/4$ |
| Fig. 3 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Fig. 4 | $\pi/2$ | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Fig. 5 | π | $\pi/3$ | π | $\pi/6$ | $\pi/2$ | $\pi/2$ | $\pi/6$ | $\pi/2$ |
| Fig. 6 | 0 | $\pi/2$ | 0 | $\pi/2$ | 0 | 0 | 0 | $\pi/4$ |
| Fig. 7 | $\pi/2$ | 0 | 0 | $\pi/2$ | 0 | $\pi/2$ | 0 | $\pi/4$ |
| Fig. 8 | 0 | $\pi/2$ | 0 | $\pi/2$ | 0 | $\pi/6$ | $\pi/4$ | $\pi/4$ |

TABLE 1. Parameter values used in simulations of NHQW

Figure 1 reproduces the classical random walk, while Figure 2 shows the usual quantum walk.

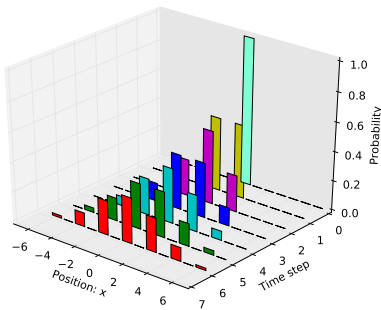


FIGURE 1. Classical random walk.

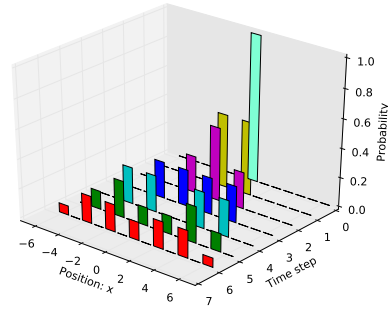


FIGURE 2. Quantum walk.

The next few walks depart significantly from the usual classical random or quantum walks. Figure 3 shows a walk in which the particle continues on its straight line trajectory it was initially set to while changing the memory qubits as it walks. Figure 4 differs from this by

flipping the $|+1\rangle$ velocity to $|-1\rangle$ at the start and then continuing with the straight line trajectory.

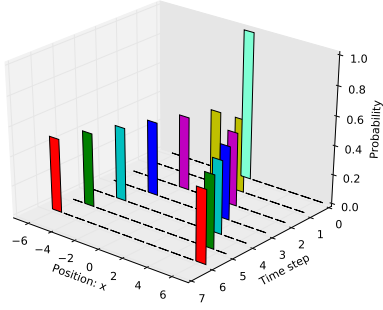


FIGURE 3.

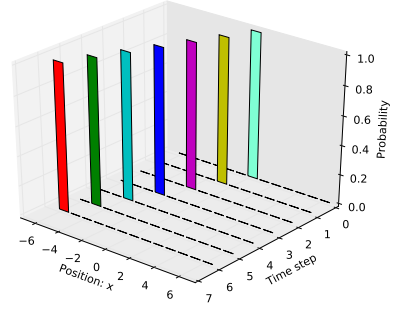


FIGURE 4.

Figures 5, 6, 7, 8, show increasingly complex patterns that result from interaction of parameters. These walks demonstrate behaviors displaying flexibility, directionality and quantum randomness.

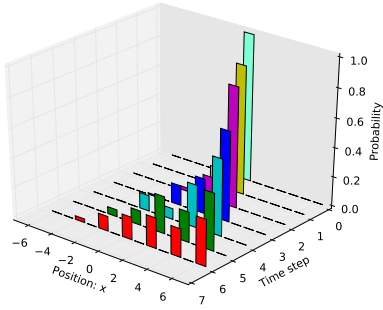


FIGURE 5.

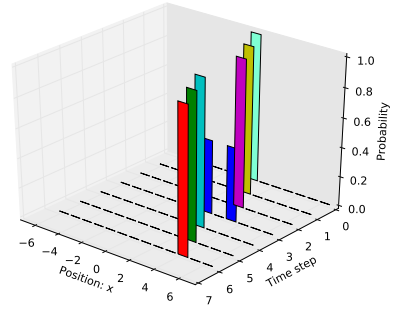


FIGURE 6.

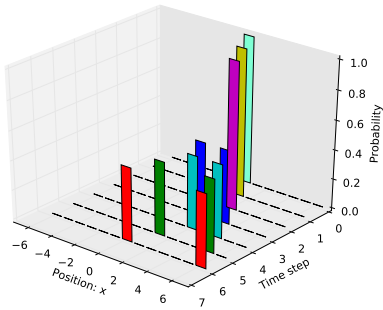


FIGURE 7.

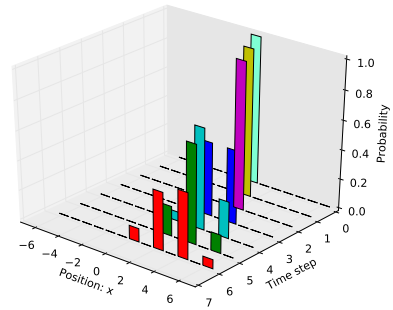


FIGURE 8.

5.3. UOB-scattering NHQW as a single-particle sector of a QCA. A quantum cellular automaton (QCA) is a discrete space, discrete time, model of physics. It consists of a collection of cells (or sites) on a lattice, each with an identical finite-dimensional Hilbert space over it, called the *cell Hilbert space*. The state of the QCA is a density operator on the Hilbert space of the QCA, which is the tensor product of the cell Hilbert spaces. The evolution of the state of the QCA is described by a *global evolution operator* that is unitary, translation-invariant and causal, i.e., restricts information to travel at a finite speed. This means that the evolution is restricted to propagate information from a cell to others within a finite *neighborhood* of it at each step of QCA evolution.

A quantum lattice gas automaton (QLGA) is a special kind of QCA, with multiple quantum particles in each cell. If we a particle may either be present or absent in a cell, it is represented by a qubit (\mathbb{C}^2), with the state $|0\rangle$ being “particle absent”, and $|1\rangle$ being “particle present”. If multiple particles are involved, the Hilbert space of a cell is a tensor product of multiple \mathbb{C}^2 factors (qubits), each of which corresponds to a particle.

The dynamics (evolution) of a QLGA consist of advection followed by scattering (or in the opposite order). These are similar, in spirit, to a QW but in a multi-particle setting. Advection, the propagation (hopping) of particles in a QLGA is a permutation of tensor factors among neighboring cell Hilbert spaces. Advection operator takes the tensor factors of a cell Hilbert space to the corresponding tensor factors of one of its neighbors, thus carrying the information about the state of particles from a cell to another. Scattering operator in a QLGA acts as an identical unitary operator on each cell Hilbert space. This cell-wise operation is said to be *local*. The reader is referred to [17, 18, 20] for the definition and examples of QCA and QLGA.

A single-particle QLGA state has one cell with a single particle in it, and the rest without a particle. The single-particle sector is the span of the single-particle states. In [18], a number of history dependent QWs were shown by construction to be the single-particle sectors of QLGA. The NHQW described in this paper, however, needs a more general description by a QCA for its multi-particle version. For a QCA, there is no natural definition of a particle. However, a cell Hilbert space may still be composed of multiple qubits, i.e., multiple \mathbb{C}^2 tensor factors. We let some of these represent particles and others represent memory qubits, a distinction that serves our purpose. A single-particle state has exactly one cell with a single particle in it, and none in the others. The span of a *subset* of single-particle states is a single-particle sector of a QCA [17].

Theorem 5.1. *The UOB-scattering NHQW is a single-particle sector of a QCA.*

Proof. We construct the QCA and its specific single-particle sector equivalent to the UOB-scattering NHQW. A cell of this QCA consists of 4 qubits, $V_0 \otimes V_1 \otimes M_0 \otimes M_1 = \bigotimes^4 \mathbb{C}^2$. Two of these $V_0, V_1 = \mathbb{C}^2$, hold the particle state as an element of $V_0 \otimes V_1$. A cell may hold none: $|v_0 v_1\rangle \in |00\rangle$, one (single): $|v_0 v_1\rangle \in \{|01\rangle, |10\rangle\}$, or two: $|v_0 v_1\rangle \in |11\rangle$, particles. The other two qubits $M_0, M_1 = \mathbb{C}^2$, hold the memory state of the cell as an element of $M_0 \otimes M_1$. A basis state of a cell is $|v_0 v_1\rangle |m_0 m_1\rangle : v_i, m_i \in \{0, 1\}$. Basis states of the QCA are $\bigotimes_{k \in \mathbb{Z}_N} |v_0^k v_1^k\rangle |m_0^k m_1^k\rangle$, where the superscript k indicates the cell index.

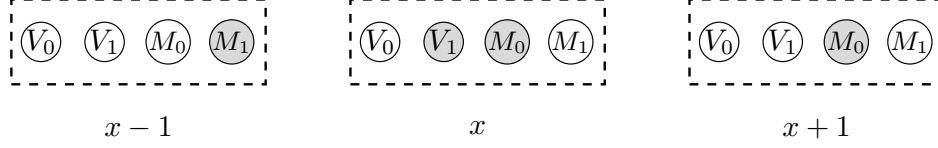


FIGURE 9. Cells of the multi-particle QCA generalizing the UOB-scattering NHQW. White circles represent $|0\rangle$. Gray circles represent $|1\rangle$.

Let us describe how the NHQW states are to be interpreted in the QCA. Each single-particle state of the cell is assigned a direction of motion: $|v_0 v_1\rangle = |01\rangle$ is right-moving and $|v_0 v_1\rangle = |10\rangle$ is left-moving. A single-particle sector of the QCA is the subspace spanned by basis states having only one cell x in a single-particle state $|v_0^x v_1^x\rangle \in \{|01\rangle, |10\rangle\}$, while the rest of the cells are in the no-particle state $|v_0^k v_1^k\rangle = |00\rangle$ for $k \neq x$. Memory qubits of the NHQW are inserted in the QCA states so as to allow the dynamics of the QCA to affect the NHQW transitions correctly. An NHQW basis state is embedded in the QCA Hilbert space as

$$\begin{aligned}
 |x\rangle | +1\rangle \otimes \bigotimes_{k \in \mathbb{Z}_N} |m_k\rangle &\longleftrightarrow \bigotimes_{k < x} |00\rangle |0m_k\rangle \otimes \underbrace{|01\rangle |m_x 0\rangle}_x \otimes \bigotimes_{k > x} |00\rangle |m_k 0\rangle, \\
 |x\rangle | -1\rangle \otimes \bigotimes_{k \in \mathbb{Z}_N} |m_k\rangle &\longleftrightarrow \bigotimes_{k < x} |00\rangle |0m_k\rangle \otimes \underbrace{|10\rangle |m_x 0\rangle}_x \otimes \bigotimes_{k > x} |00\rangle |m_k 0\rangle.
 \end{aligned} \tag{5}$$

Evolution of this QCA consists of three QLGA in tandem. We denote the first QLGA's (stage 1) advection as σ_1 and scattering as S_1 . It uses σ_1 to shuffle the neighboring memory elements to the center cell.

$$\sigma_1 : \bigotimes_{k \in \mathbb{Z}_N} |m_0^k\rangle |m_1^k\rangle \mapsto \bigotimes_{k \in \mathbb{Z}_N} |m_0^{k+1}\rangle |m_1^{k-1}\rangle,$$

acting as identity on the V_1, V_2 factors of each cell. Then S_1 acts cell-by-cell, restricting to each cell as a local (cell-wise) scattering L_1 that mimics the NHQW neighborhood scattering operator U_S in eq. (4). The scattering, U_S , of the NHQW carries over to the local scattering, L_1 , of the QLGA, through replacing the velocity states of NHQW, $|+1\rangle, |-1\rangle$, with the right/left moving states $|01\rangle, |10\rangle \in V_0 \otimes V_1$ of the QCA, respectively. The spin-transformation with parameter η in eq. (3) acts on $\{|01\rangle, |10\rangle\}$ as

$$\begin{aligned}
 |01\rangle_\eta &= \cos \eta |01\rangle + i \sin \eta |10\rangle, \\
 |10\rangle_\eta &= i \sin \eta |01\rangle + \cos \eta |10\rangle.
 \end{aligned}$$

We now get a straightforward description of the first local scattering L_1 that acts as the NHQW neighborhood scattering operator U_S ,

$$\begin{aligned}
L_1 : V_0 \otimes V_1 \otimes M_0 \otimes M_1 &\mapsto V_0 \otimes V_1 \otimes M_0 \otimes M_1 \\
|01\rangle |00\rangle &\mapsto \cos \theta_0 |01\rangle_{\alpha_0} |0\rangle_{\gamma_l} |1\rangle_{\gamma_r} + i \sin \theta_0 |10\rangle_{\alpha_1} |1\rangle_{\gamma_l} |0\rangle_{\gamma_r}, \\
|10\rangle |00\rangle &\mapsto i \sin \theta_0 |01\rangle_{\alpha_0} |0\rangle_{\gamma_l} |1\rangle_{\gamma_r} + \cos \theta_0 |10\rangle_{\alpha_1} |1\rangle_{\gamma_l} |0\rangle_{\gamma_r}, \\
|01\rangle |01\rangle &\mapsto |10\rangle_{\beta_0} |1\rangle_{\gamma_l} |1\rangle_{\gamma_r}, \\
|10\rangle |10\rangle &\mapsto |01\rangle_{\beta_0} |1\rangle_{\gamma_l} |1\rangle_{\gamma_r}, \\
|01\rangle |10\rangle &\mapsto |01\rangle_{\beta_1} |0\rangle_{\gamma_l} |0\rangle_{\gamma_r}, \\
|10\rangle |01\rangle &\mapsto |10\rangle_{\beta_1} |0\rangle_{\gamma_l} |0\rangle_{\gamma_r}, \\
|01\rangle |11\rangle &\mapsto \cos \theta_1 |01\rangle_{\alpha_1} |1\rangle_{\gamma_l} |0\rangle_{\gamma_r} + i \sin \theta_1 |10\rangle_{\alpha_0} |0\rangle_{\gamma_l} |1\rangle_{\gamma_r}, \\
|10\rangle |11\rangle &\mapsto i \sin \theta_1 |01\rangle_{\alpha_1} |1\rangle_{\gamma_l} |0\rangle_{\gamma_r} + \cos \theta_1 |10\rangle_{\alpha_0} |0\rangle_{\gamma_l} |1\rangle_{\gamma_r}.
\end{aligned}$$

The scattering operator S_1 of stage 1 QLGA acts by L_1 on each cell, so it is:

$$S_1 = \bigotimes_{k \in \mathbb{Z}_N} L_1$$

The global evolution operator for this QLGA is

$$\mathcal{G}_1 = S_1 \sigma_1.$$

The next two QLGA stages are needed to accomplish the NHQW advection⁶ and switch the memory qubits to valid positions. Stage 2 QLGA is described by the advection $\sigma_2 = \sigma_1^{-1}$ and local scattering L_2 . σ_2 takes the memory qubits from cell x (these were shuffled in from the neighbors by σ_1 , and then altered by L_1) back to the respective neighbors. In the process it also returns the memory qubits of cell x from the neighbors (unaltered).

$$\sigma_2 = \sigma_1^{-1} : \bigotimes_{k \in \mathbb{Z}_N} |m_0^k\rangle |m_1^k\rangle \mapsto \bigotimes_{k \in \mathbb{Z}_N} |m_0^{k-1}\rangle |m_1^{k+1}\rangle.$$

Stage 2 QLGA's local scattering L_2 , which sets the center cell x memory to the correct position before the next QLGA (stage 3) advection sends it to its destination (cell $x + 1$). This is needed to ensure that the memory will be in the correct form, prescribed by eq. (5), at the end of the current QCA evolution step (after stage 3 QLGA). L_2 conditionally switches the states of M_0 and M_1 if there is a right-moving particle in the cell.

$$L_2 : |01\rangle |m_0 m_1\rangle \mapsto |01\rangle |m_1 m_0\rangle.$$

It acts as identity on the other basis elements. The stage 2 scattering operator, S_2 , is

$$S_2 = \bigotimes_{k \in \mathbb{Z}_N} L_2$$

The evolution operator for this QLGA is

$$\mathcal{G}_2 = S_2 \sigma_2 = S_2 \sigma_1^{-1}$$

⁶We use the term *advection* both for a walking step of the NHQW and for the propagation of multiple particles in a QLGA.

The final stage QLGA (stage 3) first uses an advection σ_3 to carry out the NHQW advection A , hopping the particle right/left,

$$\sigma_3 : \bigotimes_{k \in \mathbb{Z}_N} |v_0^k\rangle |v_1^k\rangle \mapsto \bigotimes_{k \in \mathbb{Z}_N} |v_0^{k+1}\rangle |v_1^{k-1}\rangle,$$

while acting as identity on M_0, M_1 factors. Then it applies a local scattering L_3 , which sets the memory at the left destination cell (cell $x - 1$) to its valid state to prepare for the next QCA evolution step. It conditionally switches the states of M_0 and M_1 if there is a left-moving particle in the cell,

$$L_3 : |10\rangle |m_0 m_1\rangle \mapsto |10\rangle |m_1 m_0\rangle,$$

acting as identity on the other basis elements. This ensures that the memory will be in the correct form prescribed by eq. (5). The stage 3 scattering operator, S_3 , is

$$S_3 = \bigotimes_{k \in \mathbb{Z}_N} L_3$$

The evolution operator for stage 3 QLGA is

$$\mathcal{G}_3 = S_3 \sigma_3$$

The global QCA evolution operator, whose restriction to the single-particle sector is the NHQW transition, is

$$\mathcal{G} = \mathcal{G}_3 \mathcal{G}_2 \mathcal{G}_1 = S_3 \sigma_3 S_2 \sigma_2 S_1 \sigma_1 = S_3 \sigma_3 S_2 \sigma_1^{-1} S_1 \sigma_1. \quad (6)$$

□

In the following figures we show one step of the NHQW transition, starting with a right-moving particle state and an unbalanced neighborhood memory configuration. After the NHQW scattering counterpart S_1 , we track the projection on either the right (Figure 10) or the left-moving (Figure 11) single-particle sector, to observe the dynamics. The figures only show parts of the advection of each QLGA stage relevant to the center cell x and its neighbors, i.e., the hops in which cell x plays a part as either an origin or a destination or both during the evolution. White circles represent $|0\rangle$, gray circles represent $|1\rangle$, whereas colored circles represent any state that may be consistent with the QCA description.

Figure 10 shows the projection on the right-moving single-particle sector. After stage 2 QLGA advection, it shows the memory repositioning by stage 2 scattering S_2 in center cell x (origin). At that point, the local scattering operator L_2 (local part of S_2), acting on the center cell x , switches the M_0 and M_1 factors as the particle is in the right-moving state $|v_0^x v_1^x\rangle = |01\rangle$.

Figure 11 shows the projection on the left-moving single-particle sector. After stage 3 QLGA advection, it shows the memory repositioning by stage 3 scattering S_3 in the left cell $x - 1$ (destination). At that point, the local scattering operator L_3 (local part of S_3), acting on the left cell $x - 1$, switches the M_0 and M_1 factors as the particle is in the left-moving state $|v_0^{x-1} v_1^{x-1}\rangle = |10\rangle$.

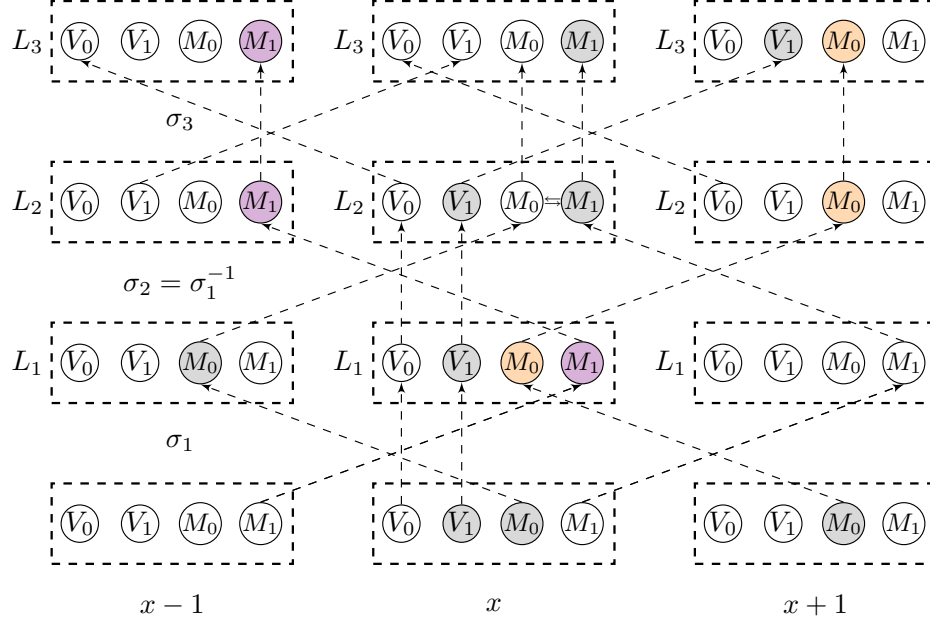


FIGURE 10. NHQW transition as a single-particle sector of the QCA. From stage 1 scattering (L_1 blocks) onwards, projection on the right-moving single-particle sector is shown. White: $|0\rangle$, gray: $|1\rangle$, colored: any state. Memory repositioning by L_2 in the origin cell x is shown by the left-right arrows.

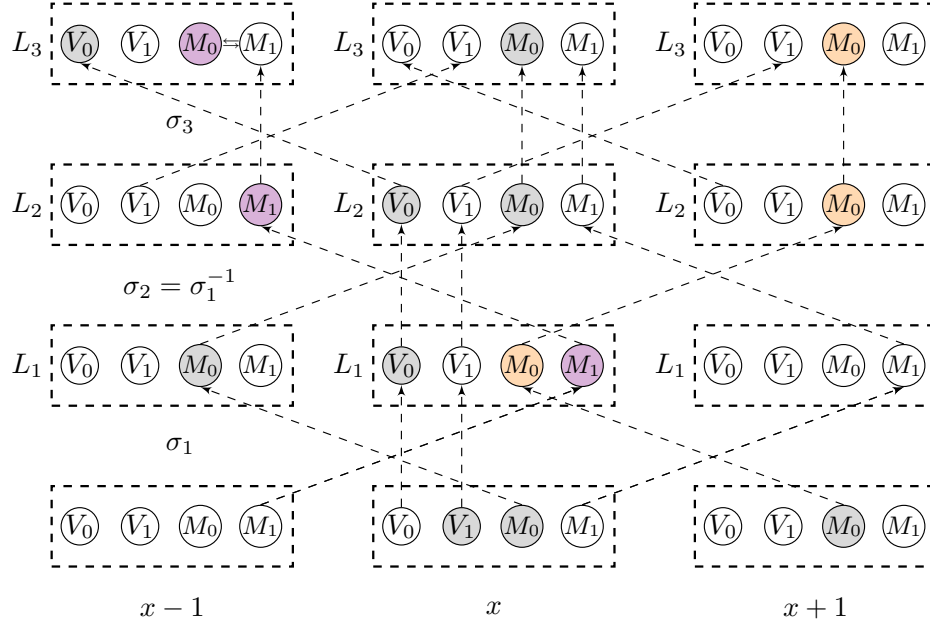


FIGURE 11. NHQW transition as a single-particle sector of the QCA. From stage 1 scattering (L_1 blocks) onwards, projection on the left-moving single-particle sector is shown. White: $|0\rangle$, gray: $|1\rangle$, colored: any state. Memory repositioning by L_3 in the destination cell $x-1$ is shown by the left-right arrows.

This QCA is a concatenation of 3 QLGA, but is not a QLGA itself when viewed at the scale at which the dynamics are homogeneous. That means that the evolution of the QCA as a whole in eq. (6) is not an advection followed by scattering acting locally on each cell, even if the cell structure were to be redefined. The analysis would be similar to that for the QCA example analyzed in [20]. In that paper, a QCA that is a concatenation of two QLGA is shown to not be a QLGA itself.

6. CONCLUSION

In this paper, we generalize an interesting model of QW from [12], that has a memory qubit at each site to keep a history of particle's visits and steer it. Our generalization allows a neighborhood of memory qubits in scattering interaction with the particle. We call it the neighborhood-history quantum walk (NHQW). We construct an example NHQW on a one-dimensional lattice, with the left/right symmetric neighboring memories. This construction utilizes unentangled orthogonal bases (UOB) [19] to define the scattering, hence we call it the UOB-scattering NHQW. The use of UOB helps in explicitly encoding the scattering strategy as a joint reconfiguration of the particle velocity and neighborhood from pre-scattering “balanced” or “unbalanced” neighborhood memory states and the particle velocity. The UOB are parametrized, so the particle velocity and the memory states undergo, upon scattering, parametrized internal (spin) state transformations. By including further “external” interaction parameters that rotate among the elements of UOB, we gain more adjustability in scattering. The scattering is geared for a reasonable search strategy. We find, through simulations, the classical random walk and quantum walk as special cases, but also several other variations in traversal patterns. These are controllable through appropriate parameter tuning. Further work in higher-dimensional lattices would reveal more fully the traversal potential of this model. We also describe a multi-particle QCA generalization of this NHQW. That QCA is a concatenation of 3 QLGA, but is not a QLGA itself. Thus, it does not have a particle description at the scale at which the dynamics are homogeneous. In this respect, our NHQW differs from a host of history dependent QWs [18], whose multi-particle generalizations are QLGA. NHQW, therefore, launches QWs into a dynamic regime with a higher degree of complexity. In the future, we aim to analyze the search capabilities and recurrence properties of NHQWs. To this end, there is an extant body of work to draw upon, concerning measures such as mixing time [21, 22], hitting time [22, 23], and Pólya Number [24].

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